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# The Kohn-Hulthén Variational Procedure for the Scattering Operator and the Reactance Operator

## Part II: Procedures Independent of the Normalization of the Trial Functions

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# THE KOHN-HULTHÉN VARIATIONAL PROCEDURE FOR THE SCATTERING OPERATOR AND THE REACTANCE OPERATOR

## Part II: Procedure Independent of the Normalization of the Trial Functions.

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July, 1956

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## Abstract

The Kohn-Hulthén variational procedures of Part I are modified so that the result for the scattering operator and reactance operator is independent of the normalization of the trial functions.

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## 1. Introduction

In Part I of this paper[1] we gave an abstract formulation of the Kohn-Hulthén variational principle. We showed

$$(1.1)\qquad {}_{o}\langle E,a|T_{-}|E,a'\rangle_{o} \cong \lim_{\nu\to 0}\ {}_{+t}\langle E+\nu,a|H-E|E,a'\rangle_{-t} + {}_{o}\langle E,a|T_{-t}|E,a'\rangle_{o}\,,$$

$$(1.2)\qquad {}_{o}\langle E,a|T_{s}|E,a'\rangle_{o} \cong \lim_{\nu\to 0}\ {}_{st}\langle E+\nu,a|H-E|E,a'\rangle_{st} + {}_{o}\langle E,a|T_{st}|E,a'\rangle_{o}\,,$$

where the states $|E,a\rangle_{\pm t}$ approximate $|E,a\rangle_{\pm}$ and $|E,a\rangle_{st}$ approximates $|E,a\rangle_{s}$, and these states are required to satisfy the conditions

$$(1.3)\quad \begin{cases} \lim\limits_{t\to -\infty} e^{iH_{o}t}\, e^{-iEt}\, |E,a\rangle_{-t} = |E,a\rangle_{o}\,, \\[2ex] \lim\limits_{t\to +\infty} e^{iH_{o}t}\, e^{-iEt}\, |E,a\rangle_{-t} = |E,a\rangle_{o} - 2\pi i \displaystyle\int |E,a''\rangle_{o}\, da''\ {}_{o}\langle E,a''|T_{-t}|E,a\rangle_{o}\,, \end{cases}$$

$$(1.4)\quad \begin{cases} \lim\limits_{t\to +\infty} e^{iH_{o}t}\, e^{-iEt}\, |E,a\rangle_{+t} = |E,a\rangle_{o}\,, \\[2ex] \lim\limits_{t\to -\infty} e^{iH_{o}t}\, e^{-iEt}\, |E,a\rangle_{+t} = |E,a\rangle_{o} + 2\pi i \displaystyle\int |E,a''\rangle_{o}\, da''\ {}_{o}\langle E,a''|T_{+t}|E,a\rangle_{o}\,, \end{cases}$$

$$(1.5)\quad \begin{cases} \lim\limits_{t\to-\infty} e^{iH_0 t} e^{-iEt} \,|E,a>_{st} = |E,a>_0 + i\pi \displaystyle\int |E,a''>_0 \, da'' \, {}_0< E,a''|T_{st}|E,a>_0 , \\[2ex] \lim\limits_{t\to+\infty} e^{iH_0 t} e^{-iEt} \,|E,a>_{st} = |E,a>_0 - i\pi \displaystyle\int |E,a''>_0 \, da'' \, {}_0< E,a''|T_{st}|E,a>_0 , \end{cases}$$

where ${}_0< E,a|T_{st}|E,a'>_0$ and ${}_0< E,a|T_{\pm t}|E,a'>_0$ approximate ${}_0< E,a|T_s|E,a'>_0$ and ${}_0< E,a|T_{\pm}|E,a'>_0$ respectively. The conditions (1.3) - (1.5) follow from the analogous conditions on $W_{\pm t}$ and $W_{st}$ (Part I, (8.2), (8.3), (8.13)) if we write

$$(1.6)\quad \begin{cases} |E,a>_{\pm t} = W_{\pm t}|E,a>_0 , \\[1ex] |E,a>_{st} = W_{st}|E,a>_0 . \end{cases}$$

Let us take as the test states $|E,a>_{\pm t}$ and $|E,a>_s$

$$(1.7)\quad \begin{cases} |E,a>_{\pm t} = |E,a>_0 + \lambda_{\pm}|E,a>^{(1)}_{\pm t} , \\[1ex] {}_0< E,a|T_{-t}|E,a'>_0 = \lambda_- \, {}_0< E,a|T^{(1)}_{-t}|E,a'>_0 , \end{cases}$$

$$(1.8)\quad \begin{cases} |E,a>_{st} = |E,a>_0 + \lambda \, |E,a>^{(1)}_{st} , \\[1ex] {}_{st}< E,a| = {}_0< E,a| + \mu \, {}^{(1)}_{st}< E,a| , \\[1ex] {}_0< E,a|T_{st}|E,a'>_0 = \lambda \, {}_0< E,a|T^{(1)}|E,a'>_0 . \end{cases}$$

where $|E,a>^{(1)}_{st}$, $|E,a>^{(1)}_{\pm}$ are arbitrary

Then on substituting (1.7) into (1.1) and minimizing with respect to $\lambda_+$ and $\lambda_-$ and on substituting (1.8) into (1.2) and minimizing with respect to $\lambda$ and $\mu$, one can obtain another form for these variational expressions. They are given in the next section.*

## 2. Alternate form for the variational expressions

Using the procedure described above we find that we can write

$$(2.1)\qquad {}_o\langle E,a|T_-|E,a'\rangle_o \cong {}_o\langle E,a|V|E,a'\rangle_o - \frac{{}_o\langle E,a|I_2|E,a'\rangle_o\left[{}_o\langle E,a|I_1|E,a'\rangle_o + {}_o\langle E,a|T_{-t}|E,a'\rangle_o\right]}{{}_o\langle E,a|I_3|E,a'\rangle_o}$$

where

$$(2.2)\qquad \begin{cases} {}_o\langle E,a|I_1|E,a'\rangle_o = \lim\limits_{\nu\to 0}\, {}_o\langle E+\nu,a|H-E|E,a'\rangle_{-r}, \\ {}_o\langle E,a|I_2|E,a'\rangle_o = {}_{+r}\langle E,a|V|E,a'\rangle_o, \\ {}_o\langle E,a|I_3|E,a'\rangle_o = \lim\limits_{\nu\to 0}\, {}_{+r}\langle E+\nu,a|H-E|E,a'\rangle_{-r}. \end{cases}$$

The states $|E,a\rangle_{\pm r}$ are to be regarded as trial functions. They are defined by

$$(2.3)\qquad |E,a\rangle_{\pm t} = |E,a\rangle_o + |E,a\rangle_{\pm r}$$

---

*Rosenberg and Spruch[2] obtained similar results for special cases of scattering. Moe and Saxon[3] also appear to have obtained similar results for special cases.

and represent the scattered (or 'radiated') waves at finite time.

From (2.1) and (2.2) it is clear that if $|E,a\rangle_{+r}$ is multiplied by any constant c and $|E,a\rangle_{-r}$ and ${}_o\langle E,a|T_{-t}|E,a'\rangle_o$ are multiplied by any other constant d, one will obtain the same approximate expression for ${}_o\langle E,a|T_-|E,a'\rangle_o$. In this sense, the variational expression (2.1) is independent of the normalization of the trial function.

One can also express $I_1$, $I_2$, $I_3$ in terms of the original trial functions $|E,a\rangle_{\pm t}$, instead of $|E,a\rangle_{\pm r}$. The expressions become

$$(2.4)\quad \begin{cases} {}_o\langle E,a|I_1|E,a'\rangle_o = \lim\limits_{\nu\to 0}\ {}_o\langle E+\nu,a|H-E|E,a'\rangle_{-t} - {}_o\langle E,a|V|E,a'\rangle_o\,, \\[2ex] {}_o\langle E,a|I_2|E,a'\rangle_o = {}_{+t}\langle E,a|V|E,a'\rangle_o - {}_o\langle E,a|V|E,a'\rangle_o \\[2ex] {}_o\langle E,a|I_3|E,a'\rangle_o = \lim\limits_{\nu\to 0}\Big\{ {}_{+t}\langle E+\nu,a|H-E|E,a'\rangle_{-t} - {}_o\langle E+\nu,a|H-E|E,a'\rangle_{-t} \\[1ex] \qquad\qquad - {}_{+t}\langle E,a|V|E,a'\rangle_o + {}_o\langle E,a|V|E,a'\rangle_o \Big\}\,. \end{cases}$$

Still another form for the variational expression (2.1) can be obtained. Equations (1.3) and (1.4) imply that $|E,a\rangle_{\pm t}$ may be written as

$$(2.5)\quad \begin{cases} |E,a\rangle_{\pm t} = |E,a\rangle_o + \gamma_\pm(E-H_o)V|E,a\rangle_{\pm v}\,, \\[2ex] {}_o\langle E,a|T_{-t}|E,a'\rangle_o = {}_o\langle E,a|V|E,a'\rangle_{-v} \end{cases}$$

where the states $|E,a\rangle_{\pm v}$ are essentially arbitrary. Then (2.1) becomes

$$(2.6)\qquad {}_{0}\langle E,a|T_{-}|E,a'\rangle_{0} \cong {}_{0}\langle E,a|V|E,a'\rangle_{0} - \frac{{}_{+v}\langle E,a|V\gamma_{-}(E-H_{0})V|E,a'\rangle_{0} \cdot {}_{0}\langle E,a|V\gamma_{-}(E-H_{0})V|E,a'\rangle_{-v}}{\left[{}_{+v}\langle E,a|V\gamma_{-}(E-H_{0})V\gamma_{-}(E-H_{0})V|E,a'\rangle_{-v} - {}_{+v}\langle E,a|V\gamma_{-}(E-H_{0})V|E,a'\rangle_{-v}\right]},$$

where now the states $|E,a\rangle_{\pm v}$ are to be regarded as the trial functions. The variational principle is clearly independent of the normalization of $|E,a\rangle_{\pm v}$. In fact, it closely resembles the usual form of the Schwinger variational principle.

One can obtain similar results for the variational principle for the reactance operator. The analogue of (2.1) is

$$(2.7)\qquad {}_{0}\langle E,a|T_{s}|E,a'\rangle_{0} \cong {}_{0}\langle E,a|V|E,a'\rangle_{0} - \frac{{}_{0}\langle E,a|\hat{I}_{2}|E,a'\rangle_{0}\left[{}_{0}\langle E,a|\hat{I}_{1}|E,a'\rangle_{0} + {}_{0}\langle E,a|T_{st}|E,a'\rangle_{0}\right]}{{}_{0}\langle E,a|\hat{I}_{3}|E,a'\rangle_{0}}$$

where

$$(2.8)\qquad \begin{cases} {}_{0}\langle E,a|\hat{I}_{1}|E,a'\rangle_{0} = \lim\limits_{\nu\to 0} {}_{0}\langle E+\nu,a|H-E|E,a'\rangle_{sr}, \\ {}_{0}\langle E,a|\hat{I}_{2}|E,a'\rangle_{0} = {}_{sr}\langle E,a|V|E,a'\rangle_{0}, \\ {}_{0}\langle E,a|\hat{I}_{3}|E,a'\rangle_{0} = \lim\limits_{\nu\to 0} {}_{sr}\langle E+\nu,a|H-E|E,a'\rangle_{sr}. \end{cases}$$

The trial state $|E,a\rangle_{sr}$ is defined by

$$(2.9)\qquad |E,a\rangle_{st} = |E,a\rangle_{o} + |E,a\rangle_{sr}\ .$$

The equations (2.8) can also be written as

$$(2.10)\quad \begin{cases} {}_{o}\langle E,a|\hat{I}_1|E,a'\rangle_{o} = \lim\limits_{\nu\to 0}\ {}_{o}\langle E+\nu,a|H-E|E,a'\rangle_{st} - {}_{o}\langle E,a|V|E,a'\rangle_{o}\ , \\[2ex] {}_{o}\langle E,a|\hat{I}_2|E,a'\rangle_{o} = {}_{st}\langle E,a|V|E,a'\rangle_{o} - {}_{o}\langle E,a|V|E,a'\rangle_{o}\ , \\[2ex] {}_{o}\langle E,a|\hat{I}_3|E,a'\rangle_{o} = \lim\limits_{\nu\to 0}\Big\{\ {}_{st}\langle E+\nu,a|H-E|E,a'\rangle_{st} - {}_{o}\langle E+\nu,a|H-E|E,a'\rangle_{st} \\[2ex] \qquad\qquad - {}_{st}\langle E,a|V|E,a'\rangle_{o} + {}_{o}\langle E,a|V|E,a'\rangle_{o}\Big\}\ . \end{cases}$$

On using the fact that $|E,a\rangle_{st}$ can always be written as

$$(2.11)\quad \begin{cases} |E,a\rangle_{st} = |E,a\rangle_{o} + \dfrac{P}{E-H_o}V|E,a\rangle_{sv}\ , \\ \text{where} \\ {}_{o}\langle E,a|T_{st}|E,a'\rangle_{o} = {}_{o}\langle E,a|V|E,a'\rangle_{sv} \end{cases}$$

and where now we regard $|E,a\rangle_{sv}$ as the arbitrary trial function, we can write equation (2.7) as

$$(2.12)\qquad {}_{o}\langle E,a|T_s|E,a'\rangle_{o} \cong {}_{o}\langle E,a|V|E,a'\rangle_{o}$$

$$- \frac{{}_{sv}\langle E,a|V\dfrac{P}{E-H_o}V|E,a'\rangle_{o}\cdot{}_{o}\langle E,a|V\dfrac{P}{E-H_o}V|E,a'\rangle_{sv}}{\left[{}_{sv}\langle E,a|V\dfrac{P}{E-H_o}V\dfrac{P}{E-H_o}V|E,a'\rangle_{sv} - {}_{sv}\langle E,a|V\dfrac{P}{E-H_o}V|E,a'\rangle_{sv}\right]}\ .$$

From (2.12) it is clear that the variational principle yields a Hermitian approximation to ${}_o\langle E,a|T_s|E,a'\rangle_o$ for all trial functions $|E,a\rangle_{st}$ or equivalently $|E,a\rangle_{sv}$.

## 3. Proof of the variational principles

The variational principles (2.1) and (2.7) were derived from simpler forms given in the Introduction. We can, however, prove these principles independently. We shall now prove (2.7); the proof of (2.1) is almost identical.

Let us first prove that when $|E,a\rangle_{st} = |E,a\rangle_s$ and ${}_o\langle E,a|T_{st}|E,a'\rangle_o = {}_o\langle E,a|T_s|E,a'\rangle_o$, the principle (2.7) gives the exact result for ${}_o\langle E,a|T_s|E,a'\rangle_o$. From (2.10) and from

$$(H-E)|E,a\rangle_s = 0 \tag{3.1}$$

it follows that

$$\left\{\begin{aligned} {}_o\langle E,a|\hat{I}_1|E,a'\rangle_o &= -\,{}_o\langle E,a|V|E,a'\rangle_o\,, \\ {}_o\langle E,a|\hat{I}_2|E,a'\rangle_o &= {}_s\langle E,a|V|E,a'\rangle_o - {}_o\langle E,a|V|E,a'\rangle_o\,, \\ {}_o\langle E,a|\hat{I}_3|E,a'\rangle_o &= -\,{}_s\langle E,a|V|E,a'\rangle_o + {}_o\langle E,a|V|E,a'\rangle_o\,. \end{aligned}\right. \tag{3.2}$$

Now, it can be shown from Part I that

$${}_s\langle E,a|V|E,a'\rangle_o = {}_o\langle E,a|T_s|E,a'\rangle_o = {}_o\langle E,a|V|E,a'\rangle_s\,. \tag{3.3}$$

Hence

(3.4) $$ {}_0\langle E,a|V|E,a'\rangle_0 - \frac{{}_0\langle E,a|\hat{I}_2|E,a'\rangle_0 \left[{}_0\langle E,a|\hat{I}_1|E,a'\rangle_0 + {}_0\langle E,a|T_s|E,a'\rangle_0\right]}{{}_0\langle E,a|\hat{I}_3|E,a'\rangle_0} $$

$$ = {}_0\langle E,a|V|E,a'\rangle_0 - \frac{\left[{}_0\langle E,a|T_s|E,a'\rangle_0 - {}_0\langle E,a|V|E,a'\rangle_0\right]^2}{-{}_0\langle E,a|T_s|E,a'\rangle_0 + {}_0\langle E,a|V|E,a'\rangle} $$

$$ = {}_0\langle E,a|V|E,a'\rangle_0 + {}_0\langle E,a|T_s|E,a'\rangle_0 - {}_0\langle E,a|V|E,a'\rangle_0 $$

$$ = {}_0\langle E,a|T_s|E,a'\rangle_0 , $$

as desired.

We shall now prove that the right-hand side of (2.7) equals ${}_0\langle E,a|T_s|E,a'\rangle_0$ to the first order in variations of $|E,a\rangle_{sv}$ about $|E,a\rangle_s$.

Let

(3.5) $$ |E,a\rangle_{sv} = |E,a\rangle_s + |E,a\rangle_1 , $$

where $|E,a\rangle_1$ is regarded as small. Then from (2.11)

(3.6) $$ |E,a\rangle_{st} = |E,a\rangle_s + \frac{P}{E-H_0} V|E,a\rangle_1 , $$

since

(3.7) $$ |E,a\rangle_s = |E,a\rangle_0 + \frac{P}{E-H_0} V|E,a\rangle_s . $$

Then from (2.10) and (3.1)

$$(3.8)\quad \left\{\begin{aligned}
{}_0\langle E,a|\hat{I}_1|E,a'\rangle_0 &= -\,{}_0\langle E,a|V|E,a\rangle_1 + {}_0\langle E,a|V\,\frac{P}{E-H_0}\,V|E,a\rangle_1 \\
&\quad -\,{}_0\langle E,a|V|E,a'\rangle_0\,, \\
{}_0\langle E,a|\hat{I}_2|E,a'\rangle_0 &= {}_s\langle E,a|V|E,a'\rangle_0 \\
&\quad +\,{}_1\langle E,a|V\,\frac{P}{E-H_0}\,V|E,a'\rangle_0 \\
&\quad -\,{}_0\langle E,a|V|E,a'\rangle_0\,, \\
{}_0\langle E,a|\hat{I}_3|E,a'\rangle_0 &= -\,{}_0\langle E,a|V\,\frac{P}{E-H_0}\,V|E,a\rangle_1 \\
&\quad -\,{}_s\langle E,a|V|E,a'\rangle_0 - {}_1\langle E,a|V\,\frac{P}{E-H_0}\,V|E,a'\rangle_0 \\
&\quad +\,{}_0\langle E,a|V|E,a'\rangle_0
\end{aligned}\right.$$

to the first order in $|E,a\rangle_1$.

Also from (2.11)

$$(3.9)\quad \begin{aligned}
{}_0\langle E,a|T_{-t}|E,a'\rangle_0 &= {}_0\langle E,a|V|E,a'\rangle_{sv} \\
&= {}_0\langle E,a|T_s|E,a'\rangle_0 + {}_0\langle E,a|V|E,a'\rangle_1\,.
\end{aligned}$$

On substituting (3.8) and (3.9) into the right-hand side of (2.7) and on using (3.3), one sees that the coefficients of terms of first order in $|E,a\rangle_1$

vanish and that the right-hand side of (2.7) is just ${}_o\!< E,a|T_s|E,a' >_o$ as is required.

## 4. The $\underset{\sim}{x}$-representation

One can easily express the variational principles in terms of the $\underset{\sim}{x}$-representation. One need merely express the operators ${}_o\!< E,a|I_1|E,a' >_o$, etc., in terms of the $\underset{\sim}{x}$-representation. The principle (2.1) and equations (2.4) become

$$(4.1)\qquad {}_o\!< E,a|T_{-}|E,a' >_o \cong \int \Psi_o^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\,\Psi_o(\underset{\sim}{x}|E,a')d\underset{\sim}{x} - \frac{{}_o\!< E,a|I_2|E,a' >_o\left[{}_o\!< E,a|I_1|E,a' >_o + {}_o\!< E,a|T_{-t}|E,a' >_o\right]}{{}_o\!< E,a|I_3|E,a' >_o},$$

where

$$(4.1a)\quad \begin{cases} {}_o\!< E,a|I_1|E,a' >_o = \lim\limits_{\nu\to 0}\displaystyle\int \Psi_o^*(\underset{\sim}{x}|E+\nu,a)(H^{\underset{\sim}{x}}-E)\,\Psi_{-r}(\underset{\sim}{x}|E,a')d\underset{\sim}{x}, \\[2ex] {}_o\!< E,a|I_2|E,a' >_o = \displaystyle\int \Psi_{+r}^*(\underset{\sim}{x}|E,a)\,V(\underset{\sim}{x})\,\Psi_o(\underset{\sim}{x}|E,a')d\underset{\sim}{x}, \\[2ex] {}_o\!< E,a|I_3|E,a' >_o = \lim\limits_{\nu\to 0}\displaystyle\int \Psi_{+r}^*(\underset{\sim}{x}|E+\nu,a)(H^{\underset{\sim}{x}}-E)\,\Psi_{-r}(\underset{\sim}{x}|E,a')d\underset{\sim}{x}. \end{cases}$$

In (4.1a) $\Psi_{\pm r}$ is defined by

$$(4.1b)\qquad \Psi_{\pm r}(\underset{\sim}{x}|E,a) = <\underset{\sim}{x}|E,a>_{\pm r} = \Psi_{\pm t}(\underset{\sim}{x}|E,a) - \Psi_o(\underset{\sim}{x}|E,a).$$

The asymptotic form of $\Psi_{-t}(\underset{\sim}{x}|E,a)$ will be an outgoing wave in which ${}_o\!< E,a|T_{-t}|E,a' >_o$ will appear as the amplitude. We require the asymptotic form of $\Psi_{+r}(\underset{\sim}{x}|E,a)$ to be an incoming wave with an arbitrary function ${}_o\!< E,a|T_{+t}|E,a' >_o$ as an amplitude.

The principle in the form (2.6) is given by

$$(4.2) \qquad {}_{o}\!\langle E,a|T_{-}|E,a'\rangle \cong \int \Psi_{o}^{*}(\underset{\sim}{x}|E,a)\, V\,(\underset{\sim}{x})\, \Psi_{o}(\underset{\sim}{x}|E,a')d\underset{\sim}{x} \;-\; \frac{AB}{C}\,,$$

where

$$(4.2a) \qquad A = \iint \phi_{+t}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{out}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\Psi_{o}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}',$$

$$(4.2b) \qquad B = \iint \Psi_{o}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{out}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{-t}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}',$$

$$(4.2c) \qquad C = \iiint \phi_{+t}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{out}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')G_{E}^{out}(\underset{\sim}{x}'|\underset{\sim}{x}'')\, V(\underset{\sim}{x}'')$$
$$\phi_{-t}(\underset{\sim}{x}''\,(E,a')d\underset{\sim}{x}d\underset{\sim}{x}'d\underset{\sim}{x}''$$
$$-\iint \phi_{+t}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{out}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{-t}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}';$$

here $\phi_{\pm t}\,(\underset{\sim}{x}|E,a)$ are essentially arbitrary functions.

The variational principle (2.7) for the reactance matrix in terms of the $\underset{\sim}{x}$-representation is

$$(4.3) \qquad {}_{o}\!\langle E,a|T_{s}|E,a'\rangle_{o} \cong \int \Psi_{o}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\Psi_{o}(\underset{\sim}{x}|E,a')d\underset{\sim}{x}$$
$$-\;\frac{{}_{o}\!\langle E,a|\hat{I}_{3}|E,a'\rangle_{o}\left[{}_{o}\!\langle E,a|\hat{I}_{1}|E,a'\rangle_{o} + {}_{o}\!\langle E,a|T_{st}|E,a'\rangle_{o}\right]}{{}_{o}\!\langle E,a|\hat{I}_{3}\,|E,a'\rangle_{o}}\,,$$

where

$$(4.3a)\quad \begin{cases} {}_{0}\langle E,a|\hat{I}_1|E,a'\rangle_{0} = \lim\limits_{\nu\to 0}\int \Psi_{0}^{*}(\underset{\sim}{x}|E+\nu,a)(H^{\underset{\sim}{x}}-E)\Psi_{sr}(\underset{\sim}{x}|E,a')\ d\underset{\sim}{x}\ , \\ {}_{0}\langle E,a|\hat{I}_2|E,a'\rangle_{0} = \int \Psi_{sr}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\Psi_{0}(\underset{\sim}{x}|E,a')d\underset{\sim}{x}, \\ \langle E,a|\hat{I}_3|E,a'\rangle = \lim\limits_{\nu\to 0}\int \Psi_{sr}^{*}(\underset{\sim}{x}|E+\nu,a)(H^{\underset{\sim}{x}}-E)\Psi_{sr}(\underset{\sim}{x}|E,a')d\underset{\sim}{x}. \end{cases}$$

In (4.3a) we have

$$(4.3b)\qquad \Psi_{sr}(\underset{\sim}{x}|E,a) = \langle \underset{\sim}{x}|E,a\rangle_{sr} = \Psi_{st}(\underset{\sim}{x}|E,a) - \Psi_{0}(\underset{\sim}{x}|E,a).$$

Asymptotically $\Psi_{sr}(\underset{\sim}{x}|E,a)$ will be a linear combination of outgoing and measuring waves with amplitudes ${}_{0}\langle E,a|T_{st}|E,a'\rangle_{0}$.

The variational principle (2.12) becomes

$$(4.4)\qquad {}_{0}\langle E,a|T_{s}|E,a'\rangle_{0} \cong \int \Psi_{0}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\Psi_{0}(\underset{\sim}{x}|E,a') - \frac{\hat{A}\,\hat{B}}{\hat{C}}$$

where

$$(4.4a)\qquad \hat{A} = \iint \phi_{st}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{S}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\Psi_{0}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}',$$

$$(4.4b)\qquad \hat{B} = \iint \Psi_{0}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{S}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{st}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}',$$

$$(4.4c)\qquad \hat{C} = \iiint \phi_{st}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{S}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')G_{E}^{S}(\underset{\sim}{x}'|\underset{\sim}{x}'')V(\underset{\sim}{x}'')\,\phi_{st}(\underset{\sim}{x}''|E,a')d\underset{\sim}{x}d\underset{\sim}{x}'d\underset{\sim}{x}''$$

$$- \iint \phi_{st}^{*}(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_{E}^{S}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{st}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}'.$$

## 5. Special cases of the x-representation

We shall now discuss the special cases treated in Part I. All notation, unless indicated otherwise, is that used in the corresponding cases of Part I. We shall restrict ourselves to the principles in the form (2.1) and (2.7).

### A. The Radial Equation with Zero Angular Momentum.

In this case we have

$$
\begin{aligned}
{}_0\langle E|T_-|E\rangle_0 &\cong \frac{1}{\pi k}\int_0^\infty \sin^2 kr\, V(r)dr \\
&\quad - \frac{{}_0\langle k|I_2|k\rangle_0}{{}_0\langle k|I_3|k\rangle_0}\left[\frac{1}{2k}\langle k|I_1|k\rangle + {}_0\langle k|T_{-t}|k\rangle\right],
\end{aligned}
\tag{5.1}
$$

where

$$
\left\{
\begin{aligned}
{}_0\langle k|I_1|k\rangle_0 &= \lim_{k'\to k}\sqrt{\frac{2}{\pi}}\int_0^\infty \sin k'r\left[\frac{-d^2}{dr^2}+V(r)-k^2\right]\Psi_{-r}(r|k)dr, \\
{}_0\langle k|I_2|k\rangle_0 &= \sqrt{\frac{2}{\pi}}\int_0^\infty \Psi^*_{+r}(r|k)V(r)\sin kr\, dr, \\
{}_0\langle k|I_3|k\rangle_0 &= \lim_{k'\to k}\int_0^\infty \Psi^*_{+r}(r|k')\left[\frac{-d^2}{dr^2}+V(r)-k^2\right]\Psi_{-r}(r|k)dr, \\
E &= k^2.
\end{aligned}
\right.
\tag{5.1a}
$$

In (5.1a) the subscript r is not to be confused with the radial coordinate r. The subscript r (for 'radiated') refers to the part of the trial function which is the scattered wave. In fact $\Psi_{\pm r}(r|k)$ are any functions which have the asymptotic form (cf. Part I, (3.11)).

$$
\lim_{r\to\infty}\Psi_{\pm r}(r|k) = -\sqrt{2\pi}\, e^{\mp ikr}\, {}_0\langle E|T_{\pm t}|E\rangle_0 .
\tag{5.1b}
$$

The variational principle for the reactance operator is

$$\tag{5.2} {}_0\langle E|T_s|E\rangle \cong \frac{1}{\pi k}\int_0^\infty \sin^2 kr\,V(r)\,dr - \frac{{}_0\langle k|\hat{I}_2|k\rangle_0}{{}_0\langle k|\hat{I}_3|k\rangle_0}\left[\frac{1}{2k}\,{}_0\langle k|\hat{I}_1|k\rangle_0 + {}_0\langle E|T_{st}|E\rangle_0\right],$$

where

$$\tag{5.2a} \begin{cases} {}_0\langle k|\hat{I}_1|k\rangle_0 = \lim\limits_{k'\to k} \sqrt{\frac{2}{\pi}} \displaystyle\int_0^\infty \sin k'r \left[-\frac{d^2}{dr^2} + V(r) - k^2\right]\Psi_{sr}(r|k)\,dr, \\ \\ {}_0\langle k|\hat{I}_2|k\rangle_0 = \sqrt{\frac{2}{\pi}} \displaystyle\int_0^\infty \Psi^*_{sr}(r|k)V(r)\sin kr\,dr, \\ \\ {}_0\langle k|\hat{I}_3|k\rangle_0 = \lim\limits_{k'\to k} \displaystyle\int_0^\infty \Psi^*_{sr}(r|k')\left[-\frac{d^2}{dr^2} + V(r) - k^2\right]\Psi_{sr}(r|k)\,dr. \end{cases}$$

The trial function $\Psi_{sr}(r|k)$ is required to satisfy

$$\tag{5.2b} \lim_{r\to\infty} \Psi_{sr}(r|k) = -\sqrt{2\pi}\cos kr\;{}_0\langle E|T_{st}|E\rangle_0 .$$

## B. The One-Dimensional Scattering Problem.

In this case we have

$$(5.3)\quad {}_0\langle E,a|T_-|E,b\rangle_0 \cong \lim_{|k'|\to|k|}\left\{\frac{1}{4\pi|k|}\int_{-\infty}^{+\infty} e^{-ik'x}\,V(x)e^{ikx}dx - \frac{{}_0\langle k'|I_2|k\rangle_0}{{}_0\langle k'|I_3|k\rangle_0}\left[\frac{1}{2|k|}\,{}_0\langle k'|I_1|k\rangle_0 + {}_0\langle E,a|T_{-t}|E,b\rangle_0\right]\right\},$$

where

$$(5.3a)\quad \begin{cases} {}_0\langle k'|I_1|k\rangle_0 = \dfrac{1}{\sqrt{2\pi}}\displaystyle\int_{-\infty}^{+\infty} e^{-ik'x}\left[-\frac{d^2}{dx^2}+V(x)-k^2\right]\Psi_{-r}(x|k)dx, \\[2ex] {}_0\langle k'|I_2|k\rangle_0 = \dfrac{1}{\sqrt{2\pi}}\displaystyle\int_{-\infty}^{+\infty} \Psi^*_{+r}(x|k')V(x)e^{ikx}dx, \\[2ex] {}_0\langle k'|I_3|k\rangle_0 = \displaystyle\int_{-\infty}^{+\infty} \Psi^*_{+r}(x|k')\left[-\frac{d^2}{dx^2}+V(x)-k^2\right]\Psi_{+r}(x|k)dx, \\[2ex] E = k^2,\ a = \dfrac{k'}{|k'|},\ b = \dfrac{k}{|k|}. \end{cases}$$

The functions $\Psi_{\pm r}(x|k)$ should satisfy the asymptotic conditions

$$(5.3b)\quad \lim_{|x|\to\infty}\Psi_{\pm r}(x|k) = \pm\sqrt{2\pi}\,i\,e^{\mp i|k||x|}\,{}_0\langle E,\mp b|T_{\pm t}|E,a\rangle_0,$$

where $E = k^2$, $a = \dfrac{k}{|k|}$, $b = \dfrac{x}{|x|}$.

For the reactance operator the principle is

$$(5.4)\qquad {}_o\langle E,a|T_s|E,b\rangle_o \cong \lim_{|k'|\to|k|}\left\{\frac{1}{4\pi|k|}\int_{-\infty}^{+\infty} e^{-ik'x}\,V(x)e^{ikx}dx - \frac{{}_o\langle k'|\hat{I}_2|k\rangle_o}{{}_o\langle k'|\hat{I}_3|d\rangle_o}\left[\frac{1}{2|k|}\,{}_o\langle k'|\hat{I}_1|k\rangle_o + {}_o\langle E,a|T_{st}|E,b\rangle_o\right]\right\},$$

where

$$(5.4a)\qquad \left\{\begin{aligned}
{}_o\langle k'|\hat{I}_1|k\rangle_o &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-ik'x}\left[\frac{-d^2}{dx^2}+V(x)-k^2\right]\Psi_{sr}(x|k)dx,\\
{}_o\langle k'|\hat{I}_2|k\rangle_o &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi^*_{sr}(x|k')V(x)e^{ikx}dx,\\
{}_o\langle k'|\hat{I}_3|k\rangle_o &= \int_{-\infty}^{+\infty}\Psi^*_{sr}(x|k')\left[-\frac{d^2}{dx^2}+V(x)-k^2\right]\Psi_{sr}(x|k)dx\\
E &= k^2,\quad a = \frac{k'}{|k'|},\quad b = \frac{k}{|k|}\,.
\end{aligned}\right.$$

In (5.4a) we require

$$(5.4b)\qquad \lim_{|x|\to\infty}\Psi_{sr}(x|k) = -\sqrt{\frac{\pi}{2}}\,i\left\{e^{i|k||x|}\,{}_o\langle E,b|T_{st}|E,a\rangle_o - e^{-i|k||x|}\,{}_o\langle E,-b|T_{st}|E,a\rangle_o\right\},$$

where $E = k^2$, $a = \dfrac{k}{|k|}$, $b = \dfrac{x}{|x|}$.

C. The Three-Dimensional Scattering Problem.

In this case,

$$
\begin{aligned}
{}_o\langle E,\theta',\phi'|T_-|E,\theta,\phi\rangle_o \cong \lim_{|\underset{\sim}{k}'|\to|\underset{\sim}{k}|}
&\cdot\left\{\frac{|\underset{\sim}{k}|}{2(2\pi)^3}(\sin\theta\,\sin\theta')^{1/2}\int e^{-i\,\underset{\sim}{k}'\cdot\underset{\sim}{x}}\,V(\underset{\sim}{x})e^{i\,\underset{\sim}{k}\cdot\underset{\sim}{x}}d\underset{\sim}{x}\right.\\
&-\frac{{}_o\langle \underset{\sim}{k}'|I_2|\underset{\sim}{k}\rangle_o}{{}_o\langle \underset{\sim}{k}'|I_3|\underset{\sim}{k}\rangle_o}\left[\frac{|\underset{\sim}{k}|}{2}(\sin\theta\,\sin\theta')^{1/2}\,{}_o\langle \underset{\sim}{k}'|I_1|\underset{\sim}{k}\rangle_o\right.\\
&\left.\left.+\,{}_o\langle E,\theta',\phi'|T_{-t}|E,\theta,\phi\rangle_o\right]\right\},
\end{aligned}
\tag{5.5}
$$

where

$$
\left\{
\begin{aligned}
{}_o\langle \underset{\sim}{k}'|I_1|\underset{\sim}{k}\rangle_o &= \frac{1}{(2\pi)^{3/2}}\int e^{-i\underset{\sim}{k}'\cdot\underset{\sim}{x}}\left[-\nabla^2+V(\underset{\sim}{x})-|\underset{\sim}{k}|^2\right]\Psi_{-r}(\underset{\sim}{x}|\underset{\sim}{k})d\underset{\sim}{x}\,,\\
{}_o\langle \underset{\sim}{k}'|I_2|\underset{\sim}{k}\rangle_o &= \frac{1}{(2\pi)^{3/2}}\int \Psi^*_{+r}(\underset{\sim}{x}|\underset{\sim}{k}')V(\underset{\sim}{x})e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}d\underset{\sim}{x}\,,\\
{}_o\langle \underset{\sim}{k}'|I_3|\underset{\sim}{k}\rangle_o &= \int \Psi^*_{+r}(\underset{\sim}{x}|\underset{\sim}{k}')\left[-\nabla^2+V(\underset{\sim}{x})-|\underset{\sim}{k}|^2\right]\Psi_{-r}(\underset{\sim}{x}|\underset{\sim}{k})d\underset{\sim}{x}\,;\\
&E = |\underset{\sim}{k}|^2;\ \theta,\ \phi \text{ are the polar angles of } k;\ \theta',\ \phi' \text{ are the polar angles of } \underset{\sim}{k}'.
\end{aligned}
\right.
\tag{5.5a}
$$

The requirements on $\Psi_{\pm r}(\underset{\sim}{x}|\underset{\sim}{k})$ are that these functions should have the asymptotic form

$$(5.5b)\quad \left\{ \begin{aligned} & \lim_{|\underset{\sim}{x}| \to \infty} \Psi_{-r}(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{-\sqrt{2}\pi\, e^{i|\underset{\sim}{k}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}|} (\sin\theta \sin\theta')^{-1/2} \\ & \qquad \cdot\ {}_{o}\!< E,\theta',\phi' | T_{-t} | E,\theta,\phi >_{o}, \\ & \lim_{|\underset{\sim}{x}| \to \infty} \Psi_{+r}(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{-\sqrt{2}\pi\, e^{-i|\underset{\sim}{k}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}|} (\sin\theta \sin\theta')^{-1/2} \\ & \qquad \cdot\ {}_{o}\!< E,\pi-\theta',\pi+\phi' | T_{+t} | E,\theta,\phi >_{o}; \\ & E = |\underset{\sim}{k}|^{2};\ \ \theta,\phi \text{ are the polar angles of } \underset{\sim}{k};\ \theta',\phi' \text{ are the polar angles of } \underset{\sim}{x}. \end{aligned} \right.$$

For the reactance operator the principle is

$$(5.6)\quad \begin{aligned} {}_{o}\!< E,\theta',\phi' | T_{s} | E,\theta,\phi >_{o} \cong \lim_{|\underset{\sim}{k}'| \to |\underset{\sim}{k}|} \Bigg\{ & \frac{|\underset{\sim}{k}|}{2(2\pi)^{3}} (\sin\theta \sin\theta')^{1/2} \\ & \int e^{-i\underset{\sim}{k}'\cdot\underset{\sim}{x}}\, V(\underset{\sim}{x})\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} d\underset{\sim}{x} \\ & - \frac{{}_{o}\!< \underset{\sim}{k}' | \hat{I}_{2} | \underset{\sim}{k} >_{o}}{{}_{o}\!< \underset{\sim}{k}' | \hat{I}_{3} | \underset{\sim}{k} >_{o}} \Bigg[ \frac{|\underset{\sim}{k}|}{2} (\sin\theta \sin\theta')^{1/2}\ {}_{o}\!< \underset{\sim}{k}' | \hat{I}_{1} | \underset{\sim}{k} >_{o} \\ & \qquad + {}_{o}\!< E,\theta',\phi' | T_{st} | E,\theta,\phi >_{o} \Bigg] \Bigg\}, \end{aligned}$$

where

$$
(5.6a)\quad \begin{cases}
{}_o\langle \underline{k}'|\hat{I}_1|\underline{k}\rangle_o = \dfrac{1}{(2\pi)^{3/2}}\displaystyle\int e^{-i\underline{k}'\cdot\underline{x}}\left[-\nabla^2 + V(\underline{x}) - |\underline{k}|^2\right]\Psi_{sr}(\underline{x}|\underline{k})d\underline{x}, \\[2ex]
{}_o\langle \underline{k}'|\hat{I}_2|\underline{k}\rangle_o = \dfrac{1}{(2\pi)^{3/2}}\displaystyle\int \Psi^*_{sr}(\underline{x}|\underline{k}')V(\underline{x})e^{i\underline{k}\cdot\underline{x}}d\underline{x}, \\[2ex]
{}_o\langle \underline{k}'|\hat{I}_3|\underline{k}\rangle_o = \displaystyle\int \Psi^*_{sr}(\underline{x}|\underline{k}')\left[-\nabla^2 + V(\underline{x}) - |\underline{k}|^2\right]\Psi_{sr}(\underline{x}|\underline{k})d\underline{x}\ ; \\[2ex]
E = |\underline{k}|^2;\ \theta,\emptyset \text{ are the polar angles of } \underline{k};\ \theta',\emptyset' \text{ are the polar angles of } \underline{k}'.
\end{cases}
$$

In (5.6a) we require

$$\lim_{|\underline{x}| \to \infty} \Psi_{sr}(\underline{x}|\underline{k}) = -\sqrt{\frac{\pi}{2}}\ \frac{1}{|\underline{x}|\,|\underline{k}|}\ (\sin\theta\ \sin\theta')^{-1/2}$$

$$(5.6b)\qquad \left\{{}_o\langle E,\theta',\emptyset'|T_{st}|E,\theta,\emptyset\rangle_o\ e^{i|\underline{k}||\underline{x}|} + {}_o\langle E,\pi-\theta',\pi+\emptyset'|T_{st}|E,\theta,\emptyset\rangle_o\ e^{-i|\underline{k}||\underline{x}|}\right\}$$

$E = |\underline{k}|^2$, $\theta,\emptyset$ are the polar angles of $\underline{k}$; $\theta',\emptyset'$ are the polar angles of $\underline{k}'$.

D. Scattering of an Electron by an Atom

Now we have

$$
(5.7)\quad \begin{aligned}
{}_o\langle E,\theta',\emptyset',n'|T_-|E,\theta,\emptyset,n\rangle_o = \lim_{E'\to E}\Bigg\{ & \frac{1}{(2\pi)^3}\ \frac{(|\underline{k}||\underline{k}'|\sin\theta\ \sin\theta')^{1/2}}{2} \\
& \cdot \iint e^{-i\underline{k}'\cdot\underline{x}}\ \chi^*(\underline{y}|n')V(\underline{x},\underline{y})e^{i\underline{k}\cdot\underline{x}}\ \chi(\underline{y}|n)d\underline{x}d\underline{y} \\
& - \frac{{}_o\langle \underline{k}',n'|I_2|\underline{k},n\rangle_o}{{}_o\langle \underline{k}',n'|I_3|\underline{k},n\rangle_o}\left[\frac{(|\underline{k}||\underline{k}'|\sin\theta\ \sin\theta')^{1/2}}{2}\ {}_o\langle \underline{k}',n'|I_1|\underline{k},n\rangle_o \right. \\
& \left. + {}_o\langle E,\theta',\emptyset',n'|T_{-t}|E,\theta,\emptyset,n\rangle_o\right]\Bigg\},
\end{aligned}
$$

where we require

(5.7a)

$${}_0\langle \underline{k}', n' | I_1 | \underline{k}, n \rangle_0 = \frac{1}{(2\pi)^{3/2}} \iint e^{-i\underline{k}'\cdot\underline{x}} \chi^*(\underline{y}|n') \left[H - |\underline{k}|^2 - E_n\right] \Psi_{-r}(\underline{x},\underline{y}|\underline{k},n)\, d\underline{x}d\underline{y},$$

$${}_0\langle \underline{k}', n' | I_2 | \underline{k}, n \rangle_0 = \frac{1}{(2\pi)^{3/2}} \iint \Psi^*_{+r}(\underline{x},\underline{y}|\underline{k}',n') V(\underline{x},\underline{y}) e^{i\underline{k}\cdot\underline{x}} \chi(\underline{y}|n)\, d\underline{x}d\underline{y},$$

$${}_0\langle \underline{k}', n' | I_3 | \underline{k}, n \rangle_0 = \iint \Psi^*_{+r}(\underline{x},\underline{y}|\underline{k}',n') \left[H - |\underline{k}|^2 - E_n\right] \Psi_{-r}(\underline{x},\underline{y}|\underline{k},n)\, d\underline{x}d\underline{y} ;$$

$E = |\underline{k}|^2 + E_n$; $E' = |\underline{k}'|^2 + E_{n'}$; $\theta$, $\phi$ are the polar angles of $\underline{k}$;

$\theta'$ $\phi'$ are the polar angles of $\underline{k}'$;

$$H = -\nabla^2_{\underline{x}} + H^{(A)}_{\underline{y}} + V(\underline{x},\underline{y}).$$

Also

(5.7b)

$$\lim_{|\underline{x}| \to \infty} \Psi_{-r}(\underline{x},\underline{y}|\underline{k},n) = -\left(\frac{2\pi}{|\underline{k}|}\right)^{1/2} (\sin\theta \sin\theta')^{-1/2} \sum_{n'} \frac{e^{i|\underline{k}_{n'}||\underline{x}|}}{|\underline{x}||\underline{k}_{n'}|^{1/2}} \chi(\underline{y}|n')\ {}_0\langle E,\theta',\phi',n' | T_{-t} | E,\theta,\phi,n \rangle_0 ,$$

$$\lim_{|\underline{x}| \to \infty} \Psi_{+r}(\underline{x},\underline{y}|\underline{k},n) = -\left(\frac{2\pi}{|\underline{k}|}\right)^{1/2} (\sin\theta \sin\theta')^{-1/2} \sum_{n'} \frac{e^{-i|\underline{k}_{n'}||\underline{x}|}}{|\underline{x}||\underline{k}_{n'}|^{1/2}} \cdot \chi(\underline{y}|n')\ {}_0\langle E,\pi-\theta',\pi+\phi' | T_{+t} | E,\theta,\phi,n \rangle_0 ,$$

$|\underline{k}_{n'}|^2 + E_{n'} = E = |\underline{k}|^2 + E_n$; $\underline{k}_n \equiv \underline{k}$;

$\theta,\phi$ are the polar angles of $\underline{k}$; $\theta',\phi'$ are the polar angles of $\underline{x}$.

The variational principle for the reactance matrix is

$$(5.8)\qquad {}_0\langle E,\theta',\phi',n'|T_s|E,\theta,\phi,n\rangle_0 =$$

$$\lim_{E'\to E}\left\{\frac{1}{(2\pi)^3}\,\frac{(|\underset{\sim}{k}||\underset{\sim}{k}'|\sin\theta\,\sin\theta')^{1/2}}{2}\iint e^{-i\,\underset{\sim}{k}'\cdot\underset{\sim}{x}}\,\chi^*(\underset{\sim}{y}|n')\right.$$

$$\cdot V(\underset{\sim}{x},\underset{\sim}{y})e^{i\,\underset{\sim}{k}\cdot\underset{\sim}{x}}\chi(\underset{\sim}{y},n)d\underset{\sim}{x}d\underset{\sim}{y}$$

$$-\frac{{}_0\langle \underset{\sim}{k}',n'|\hat{I}_2|\underset{\sim}{k},n\rangle_0}{{}_0\langle \underset{\sim}{k}',n'|\hat{I}_3|\underset{\sim}{k},n\rangle_0}\left[\frac{(|\underset{\sim}{k}||\underset{\sim}{k}'|\sin\theta\,\sin\theta')^{1/2}}{2}\,{}_0\langle \underset{\sim}{k},n'|\hat{I}_1|\underset{\sim}{k},n\rangle_0\right.$$

$$\left.\left.+\;{}_0\langle E,\theta',\phi',n'|T_{st}|E,\theta,\phi,n\rangle_0\right]\right\}\;,$$

where

$$(5.8\text{a})\quad\left\{\begin{aligned}
&{}_0\langle \underset{\sim}{k}',n'|\hat{I}_1|\underset{\sim}{k},n\rangle_0 = \frac{1}{(2\pi)^{3/2}}\iint e^{-i\underset{\sim}{k}'\cdot\underset{\sim}{x}}\,\chi^*(\underset{\sim}{y}|n')\cdot\left[H-|\underset{\sim}{k}|^2-E_n\right]\Psi_{sr}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n)d\underset{\sim}{x}d\underset{\sim}{y},\\
&{}_0\langle \underset{\sim}{k}',n'|\hat{I}_2|\underset{\sim}{k},n\rangle_0 = \frac{1}{(2\pi)^{3/2}}\iint \Psi^*_{sr}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k}',n')V(\underset{\sim}{x},\underset{\sim}{y})e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\chi(\underset{\sim}{y}|n)d\underset{\sim}{x}d\underset{\sim}{y}\,,\\
&{}_0\langle \underset{\sim}{k}',n'|\hat{I}_3|\underset{\sim}{k},n\rangle_0 = \iint \Psi^*_{sr}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k}',n')\left[H-|\underset{\sim}{k}|^2-E_n\right]\Psi_{sr}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n)d\underset{\sim}{x}d\underset{\sim}{y}\;;\\
&E = |\underset{\sim}{k}|^2 + E_n;\quad E' = |\underset{\sim}{k}'|^2 + E_n;\quad \theta,\phi \text{ are the polar angles of } \underset{\sim}{k};\\
&\qquad \theta',\phi' \text{ are the polar angles of } \underset{\sim}{k}'.
\end{aligned}\right.$$

In (5.8a) we require

$$
(5.8b)\quad \left\{
\begin{aligned}
&\lim_{|x|\to\infty} \Psi_{sr}(\underset{\sim}{x}|\underset{\sim}{k},n) = -\left(\frac{\pi}{2|\underset{\sim}{k}|}\right)^{1/2} (\sin\theta \sin\theta')^{-1/2} \\
&\quad\cdot \sum_{n'} \chi(\underset{\sim}{y}|n') \left\{ \frac{e^{i|\underset{\sim}{k}_{n'}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}_{n'}|^{1/2}} {}_{o}\!< E,\theta',\phi',n'|T_s|E,\theta,\phi,n >_{o} \right. \\
&\qquad\qquad \left. + \frac{e^{-i|\underset{\sim}{k}_{n'}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}_{n'}|^{1/2}} {}_{o}\!< E,\pi-\theta',\pi+\phi',n'|T_s|E,\theta,\phi,n >_{o} \right\} ; \\
&\quad E = |\underset{\sim}{k}|^2 + E_n = |\underset{\sim}{k}_{n'}|^2 + E_{n'} ; \quad \underset{\sim}{k}_n \equiv \underset{\sim}{k} ; \\
&\quad \theta,\phi \text{ are the polar angles of } \underset{\sim}{k};\ \theta',\phi' \text{ are the polar angles of } \underset{\sim}{x}.
\end{aligned}
\right.
$$

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